

Deacetylmoxisylyte
35231-36-8 | DTXSID10188722

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.07e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.29e-01

Confidence level: 5.72e-01

Nearest Neighbors from the Training Set

Image not found

N-Phenyldiethanolamine

Measured: 1.84e-01

Predicted: 4.75e-01

Image not found

2-(Dibutylamino)ethanol

Measured: 2.31e-02

Predicted: 2.46e-02

Image not found

Ethanol, 2-(ethylphenylamino)-

Measured: 1.21e-02

Predicted: 6.04e-02